



Cationic variation for LnAl_2Si_2 ($\text{Ln} = \text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds by density functional theory



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ABSTRACT

Detailed Cationic variation for LnAl_2Si_2 ($\text{Ln} = \text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds have been discussed under the frame work of density functional theory (DFT). Our reported optimized theoretical lattice constants for the studied material are in good agreement with experimental measurements and we also find that ferromagnetic phase is more stabilize and acceptable in comparison with Nonmagnetic phase. The calculated band structures and density of state (DOS) of LnAl_2Si_2 show metallic nature due to the overlapping and crossing mechanisms of minima of conduction band (CB) and maxima valance band (VB) across the Fermi level as well as strong hybridization of Y d and Sm/Tb/Dy/Yb f states with (Al, Si) p states in both spin configurations. Lastly, the investigation of magnetic properties defines a strong metallic behavior for all these understudy ferromagnetic compounds. These result shows that the ternary lanthanide based aluminum silicides are likely encouraging candidates for advance future magnetic applications especially in the vast area of spintronics.

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1. Introduction

From the past few decades' researcher utilized various structure types to show that the prerequisite for formation of the CaAl_2Si_2 structure type consistence with specific conditions, such as the total number of valence electrons present in per formula unit should be less than or equal to 16 [1–3]. The main advantage to search for these intermetallic phase materials was due to their broad range innovative applications like computer read, shape memory alloys, dentistry and jewelry [4,5] along with the technological achievements whether as (C-M-R) "colossal" or (G-M-R) "giant" magneto-resistive materials with the prime mechanism like the change of resistivity with respect to external magnetic field [6–10] in metallic thin films to accomplished magneto-resistance. The formerly known Pnictide AM_2X_2 (A: electropositive Element; M: metal; X: P - Bi) follow without exemption into this idea; which initially

in contradicting associations LnLi_2X_2 ($\text{Ln}: \text{Ce}, \text{Pr}, \text{Nd}, \text{Tb}$; $\text{X}: \text{P} - \text{Bi}$) [11–13] turned out to be later to LnLi_3X_2 corrected [14]. The only known silicides LnAl_2Si_2 and germanides LnAl_2Ge_2 (Ln : trivalent rare earth metal, Y) remain [15–18], which crystallize in the CaAl_2Si_2 type, but according to e.g. $\text{Ln}^{3+}(\text{Al}^{3+})_2(\text{Si}^{4-})_2$ are not composed its valence. Since the structural data of GdAl_2Si_2 [18] rule out that the distributions of cation according to the formulas are available further the same should be the case apply for the Germanide as well, it appeared to be beneficial to us to utilize this Connections likewise as to their electronic behavior to examine the structure more closely. To begin with the silicides of trivalent rare earth metals, of which so far just a structure determination of GdAl_2Si_2 is available, while CeAl_2Si_2 [19] and YAl_2Si_2 [20] were only published the lattice constants and for sure existed in older works similar connections with $\text{Ln} = \text{Pr}, \text{Gd-Lu}$ confirmed, but otherwise no detail of crystallographic information is reported [15,16].

Five compounds LnAl_2Si_2 (Ln : trivalent rare-earth metal, Y) have been synthesized by heating the elements between 800° and 1000 °C. They are isotypic as well as crystallize in the CaAl_2Si_2

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type structure (P3/m; $Z = 1$) [21]. The electronic band structures were calculated through LMTO code for both CaAl_2Si_2 and YAl_2Si_2 , the latter one shows non-electrovalent composition with one more valence electron per formula, are discussed in that order with the help of bonding mechanisms and the electrical conductivity [21]. Further characterization of $\text{GdAl}_{2-x}\text{Mn}_x\text{Si}_2$ mixed crystals depicted, that the structure type as of now at low Mn content ($x \approx 0.3$) changes from CaAl_2Si_2 (GdAl_2Si_2) to ThCr_2Si_2 type structure (GdMn_2Si_2).

The crystallization in the same structure and space group have been done for $\text{EuAl}_2\text{Si}_2/\text{EuAl}_2\text{Ge}_2/\text{YbAl}_2\text{Ge}_2$ compounds and were manufactured by heating all the elements between 1070 and 1270 K and further characterization has been done by method of single-crystal X-ray. Both EuAl_2Si_2 and EuAl_2Ge_2 compounds reported paramagnetic behavior beyond 50 K and indicating divalent europium by measuring magnetic susceptibility. Further antiferromagnetic order is detected at Neel temperature with the values $T_N=35.5$ K and $T_N=27.5$ K for the compounds EuAl_2Si_2 and EuAl_2Ge_2 respectively [22]. The ordinary response of an intermediate valent compound YbAl_2Si_2 has been described in the temperature range from 100 to 300 K. The linear trend of inverse susceptibility relies on providing temperature with a decreased magnetic moment value of $2.57\mu_B/\text{Yb}$ along with highly reported negative paramagnetic Curie temperature of about -382 K. Under the temperature 100 K the degree of divalent ytterbium was sharply growing [22]. Further the nonmagnetic $4f^{14}$ ground states were reported in Yb based compounds, however at the fermi level the contribution of high 4f depicts the ability to create intermediate valency in YbAl_2Si_2 . Furthermore, the explanation behind their stability is a disappearing band gap when the present atoms in $\text{M}_2 \times 2$ -slabs show minor electro-negativity differences. For this situation, the surplus-electron does not take part in destabilizing the structure as it would happen when the energy gap is available. Thus it is clear that the metallic response is not only the presence of the surplus electron, simply the whole electronic structure is that of a metal itself [21]. Apart from this, each compound $\text{AAl}_2 \times 2$ with $X = \text{Si}$ or Ge and CaAl_2Si_2 structure type is likely to be metallic, in any case the valence shell electron of the base metal A.

Generally, silicide layers are fast diffusion paths for silicon point defects and other chemical elements. Due to the different linear thermal expansion coefficients of silicide materials compared to other semiconductor materials stress will be induced during thermal treatment [23]. So far by arc melting of pure elements followed by annealing temperature at about 780 K for 7 days the $\text{Dy}_8\text{Al}_{16}\text{Si}_{30}$ (DAS) alloy was synthesized. By using XRD and SEM the structural characterization of both binary and ternary silicides, DySi_2 , DyAl_2Si_2 along with Al solid solution and Si have been performed. Even after annealing the phase mixture stays unaltered [24]. Both aluminum silicides as well as aluminum germanides $\text{AAl}_2 \times 2$ ($A = \text{rare metal or alkaline earth metal}$ and $X = \text{Si or Ge}$) [25, 26] were crystallize in the composition of trigonal La_2O_3 -type structure [27], where ordered double-corrugated hexagonal layers are arranged chemically of Al and Si (Ge) atoms while intercalated A atoms are present among them. The stability showed by these compounds was surprising due to the minor electro negativity difference between the double layer atoms. In addition to this the electronic structure and electron-phonon interaction has been investigated by using density functional theory for YAl_2Si_2 compound [28]. The Fermi energy level mostly crossed by Y 4d-like conduction band while the major participation to the (DOS) density of states comes from the same Y 4d-states at the Fermi level. The reported phonon DOS along with the Eliashberg spectral function showed that bond stretching modes which observed in-plane have larger frequency and more tightly coupled to the electrons. Both the reported (EP) coupling constant $\lambda=0.31$ as well as

the noted super-conducting transition temperature T_C (0.15 K with $\mu \sim 15$) are extremely lower in YAl_2Si_2 [28].

The phenomenon of de hybridization for inter-metallic isostructural compounds of the RAl_2Si_2 ($R = \text{Sm, Eu, Gd, Tb, Er, Yb}$) row for the first time has been performed theoretically. The physical nature of the occasion of a σ -like hump, the value of which is proportional to the number of lattice sites N formed by R -Si structural elements, is also explained. In correlation with a single admixture, the value of σ -like hump increases N times [29]. This is due to the fact that the R/Si orbitals play the role of electronic defects which are periodically located within the entire crystal lattice. The performed both theoretical and experimental investigations showed a high degree of correlation and self-consistency, which allows us to consider the $R - \text{Si}$ atomic bonds as a kind of electronic defects, strongly disturbing the electronic arrangement of RAl_2Si_2 compounds. Such perturbation is displayed in the appearance of intense resonant peaks of electronic states, which are formed in the valence band of the investigated inter-metallics as a result of the action of de hybridization factor [29].

Aluminum silicide microparticles with oxidized rough surfaces were formed on Si substrates through a spontaneous granulation process of Al films. This microparticle formation was caused by interdiffusion of Al and Si atoms at hypoeutectic temperatures of Al-Si systems, which was driven by compressive stress stored in Al films. The size, density, and the composition of the microparticles could be controlled by adjusting the annealing temperature, time, and the film thickness. High-density microparticles of a size around $10 \mu\text{m}$ and with an atomic ratio of Si/Al of approximately 0.8 were obtained when a 90-nm-thick Al film on Si substrate was annealed for 9 h at 550°C . The microparticle formation resulted in a rapid increase of the sheet resistance, which is a consequence of substantial consumption of Al film. This simple route to size- and composition-controllable microparticle formation may lay a foundation stone for the thermoelectric study on Al-Si alloy-based heterogeneous systems. Thermoelectric energy generation, by which waste heat is converted into electricity, has emerged as one of key energy renewal technologies since a huge amount of world energy is wasted in the form of heat [30].

This shows that the existing literature about these compounds is still limited by different point of views and need further attention for best possible output. Regarding these compounds, there is lack of theoretical or computational data in a common family of materials, this study was assumed to find first time the basic properties such as physical, structural, electronic and magnetic for ternary lanthanide-based aluminum silicides compounds. To the best of our knowledge, there are no past data available on Cationic variation for LnAl_2Si_2 ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) compounds by density functional theory.

2. Computational details

In this research, the computational calculations have been achieved for LnAl_2Si_2 ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) compounds according to DFT [31]. The calculations were performed by means of the full potential linearized augmented plane wave (FP-LAPW) approach [32] as implemented in the WIEN2k code [33]. The exchange-correlation potentials were calculated by the help of generalized gradient approximation (GGA-PBE) [34]. PBE-GGA gives better results as compared to the LDA. The PBE-GGA approximation completely describes the inhomogeneity of an electronic system. It overcomes the limitations imposed by LDA; it also improves the description related to the binding energy of the molecules. One approach to further improve the exactness of description of d/f localized electrons is the utilization of the spin-polarised GGA+U method [35], which includes an on-site Coulomb repulsion. Further the wave functions in the interstitial region were expanded in

Table 1Calculated lattice parameters, (*a*, *c* (Å)), *B* (GPa), *B_p* and *E₀* (Ry) for ferromagnetic ternary aluminum Silicides compounds along with other theoretical results.

Compounds	Lattice <i>a</i>	Constant <i>C</i>	<i>V₀</i>	<i>B</i> (GPa)	<i>B_p</i>	<i>E₀</i> FM	NM
YAl ₂ Si ₂	4.18	6.601	739.1235	75.3311	5	-8902.922	-8902.9
Exp ^a	4.195	6.581					
SmAl ₂ Si ₂	4.05	6.85	790.6370	60.7604	5	-23,001.03	-23,000.70
Exp ^a	4.202	6.723					
TbAl ₂ Si ₂	4.04	6.95	751.3824	68.1148	5	-25,569.72	-25,569.31
Exp ^a	4.184	6.59					
DyAl ₂ Si ₂	4.2	6.8	702.9544	74.2167	5	-26,468.36	-26,467.99
Exp ^a	4.185	6.569					
YbAl ₂ Si ₂	4.1	7.1	682.5934	79.1971	5	-30,290.40	-30,290.36
Exp ^a	4.156	6.914					

^a Ref:21.

plane waves with a cut off ($K_{\max}^2 = (8/R_{\text{MT}})^2$). The muffin-tin radii (R_{MT}) are taken to be (2.5, 2.16, 1.92) a.u for (Ln, Al, Si) elements respectively. The wave functions within muffin-tin spheres were expanded in spherical-harmonics with a cut off up to $l_{\max}=10$, whereas the charge density is Fourier expanded up to $G_{\max} = 12$ atom unit (au)⁻¹. By using scalar-relativistic approach the value of $R_{\text{MT}} \times K_{\max}$ was set to 7: R_{MT} refers to the smallest muffin-tin spheres (R_{MT}) radius in the unit cell, whereas k_{\max} is the largest reciprocal lattice vector. The k integration over the Brillouin zone has considered up to 1000 k points [36, 37] in the irreducible Brillouin Zone for LnAl₂Si₂ compounds in ferromagnetic phase.

3. Results and discussion

3.1. Structural properties

In this investigation we have computed the PBE-GGA approximation for these ternary aluminum silicides compounds, such as LnAl₂Si₂ (Ln=Y, Sm, Tb, Dy, Yb), using the first-principles calculations. All the compounds crystallize in the trigonal structure with space group P3/m1 (#164). The site positions for Ln, is the Wyckoff position 1a, and for Al and Si are Wyckoff position 2d in two phases namely Ferromagnetic (FM) and Nonmagnetic (NM) the optimization processes are performed for under study materials. The structure variation of the compounds is clarified by investigating structure parameters. The lattice parameters (*a*, *c* (Å)), bulk modulus, *B*(GPa) and pressure derivative (*B'*) are obtained by volume optimization of the unit cell of LnAl₂Si₂ (Ln=Y, Sm, Tb, Dy, Yb). Fig. 1(a-e) shows the optimization curves for the reported compounds. The ground state energy is the lowest among all energies define by the unit cell, and the volume related to this optimum energy is known as ground state volume. The calculated value of these parameters is shown in Table 1. There is overall a clear decreasing trend in '*a*' and volume (*V₀*), while increasing trend in *c* (Å) as one replaces the cations from Y to Yb. Further the overall increase in *B* (GPa) from Y to Yb shows that compressibility of materials decreases when moving from left to right in the periodic table. The lowest energy state of these compounds is ferromagnetic phase as compared to PM phase by using this formula FM-PM phase. So, the studied material stabilizes in the FM phase. Furthermore, the energy calculations show the favorable nature of the FM configuration. Our calculated structural properties (See Fig. 1(a-e)) are in good agreement with the other published reports [21].

3.2. Electronic properties

3.2.1. Band structure and density of states

In this study, the electronic band structure of LnAl₂Si₂ (Ln =Y, Sm, Tb, Dy, Yb) compounds with up and down spin types are calculated by Modified Becke-Johnson exchange potential (mBJ-GGA)

scheme in Fig. 2. Band structure (BS) gives important information of electro-magnetic properties, and bonding nature as well. For ease, the Fermi level is taken as zero. Energy band structures of under studied compounds are plotted along with highly symmetry point's Γ -M-K- Γ -A of Brillouin zone (BZ).

The valence band maximum shows dominant dispersion along both basal-plane Γ -K and Γ -M directions, and most interestingly, also along the *c*-axis, the Γ -A line. This depicts that the conductivity of LnAl₂Si₂ is expected to be strong almost in all directions. In addition to this, there is another band appear at Γ for almost all the reported compounds, below but close to the valence band maxima. This kind of multiband nature near the valence band maximum (VBM) is a dominant positive characteristic for thermoelectric materials. The conduction band minima is mainly due to the Y d and Sm/Tb/Dy/Yb f characters, while the maxima of valence band is mainly compose of p character contributing from the Al/Si elements in both spin types. The broad feature of the band structures is very analogous for all the compounds in both spin states. However, there are some differences due to the more continued d orbitals appears in YAl₂Si₂, the overlap among the (Al, Si) p and the Y d orbitals turn into stronger. Therefore, the overlap is larger enough between the valence and conduction bands in YAl₂Si₂ than the rest of the other understudy compounds. One has noted that the bands have larger and wider dispersion along the Γ -A direction, reflecting active inter-layer coupling in LnAl₂Si₂ (Ln =Y, Sm, Tb, Dy, Yb). Additional noteworthy differences in the compounds band structures are the crossing mechanisms of valence/conduction bands as well as the location of the Fermi level in both spin channels.

The valence band remains below the Fermi level at the high symmetry points in both spin states of YAl₂Si₂ follow by the other understudy compounds with the opposite and peculiar trend when the valence band in SmAl₂Si₂ crosses the Fermi level and the dominant appearance of two bands in up spin at Γ is clearly observe while with the down spin, valence remains lie at the same Γ point. Further in TbAl₂Si₂ it crosses the Fermi level at only Γ in up spin while crosses the entire Fermi level in down spin and overlap with only one band in conduction band region with clear dominance at Γ whereas in DyAl₂Si₂ it lies and crosses the Fermi level at Γ point in its up and down spin channels. Furthermore, in YbAl₂Si₂ the flat valence bands appear below the Fermi with few bands crosses the Fermi level at Γ point in both spin states. At the Fermi level none of the compounds shows an energy gap, in conformity with the conductivity measurements.

In LnAl₂Si₂, the Fermi level EF shifts upward because of the addition of one more valence electron per unit cell. On the other side only one conduction band crossing the Fermi energy level at high symmetry M point appears in various band structures of both states. The valence bands are completely filled and do not hold holes. Thus, the BS of LnAl₂Si₂ show metallic nature due to

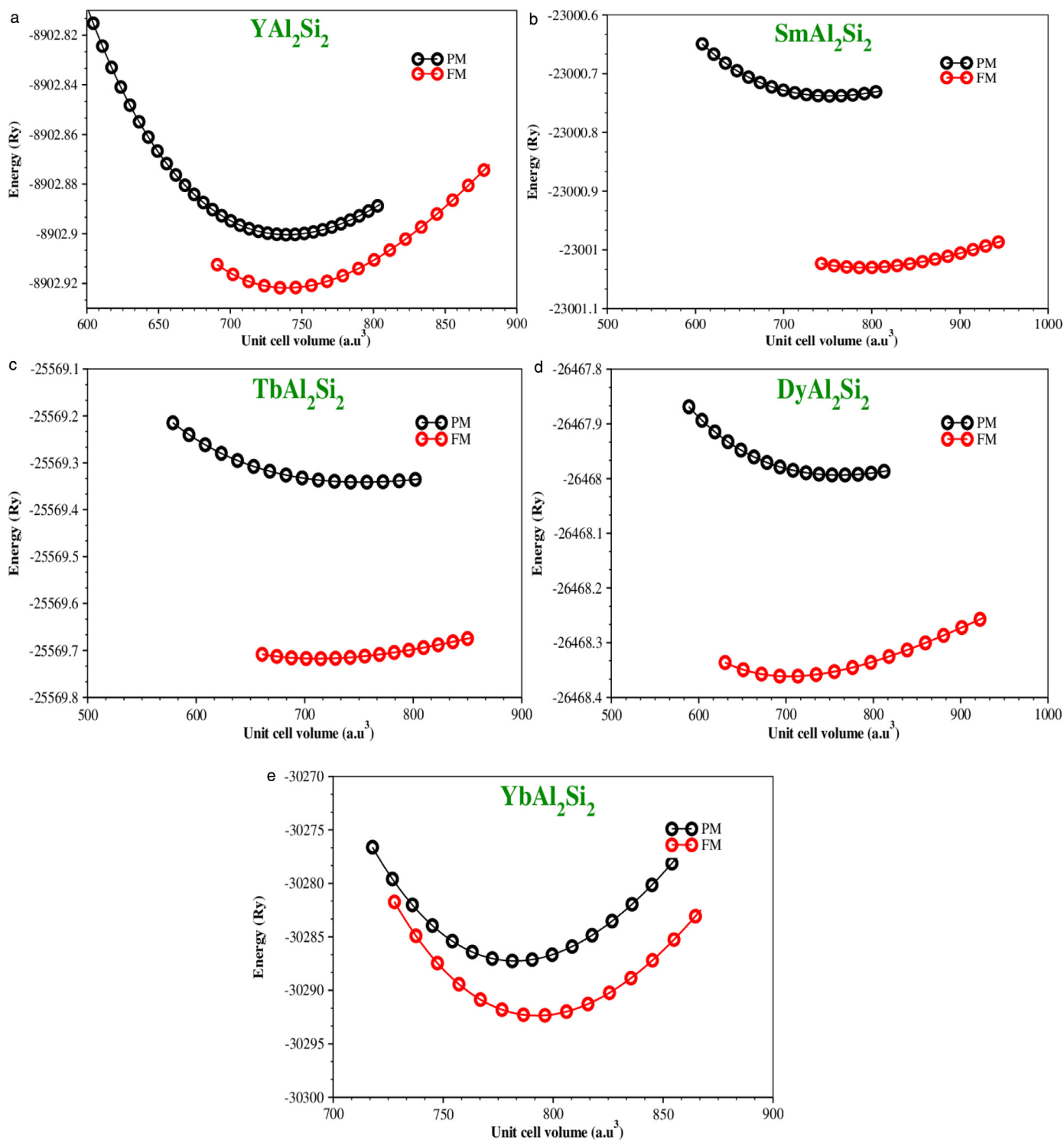


Fig. 1. (a-e): Optimization plots showing energy verses unit cell volume for LnAl_2Si_2 ($\text{Ln}=\text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds.

the overlapping and crossing mechanisms of conduction band (CB) minimum and valance band (VB) maximum across the Fermi level in both spin configurations.

Moreover, to examine about the different partial participation of (s, p, d and f) states of these compounds we have plotted total density of states (DOS) and atom partial DOS of LnAl_2Si_2 ($\text{Ln}=\text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds with both spin up and down direction are presented in Fig. 3. The LnAl_2Si_2 compounds are examined in the energy ranges from -20 to 20 eV. However, the total

density of states curves shows metallic behavior for all the under-study compounds because their partial s, p, d, f states crossing the Fermi level in both spin configurations. It can be observing from the total DOS that the dominant contribution at EF originates from Y d while Sm/Tb/Dy/Yb f states. Furthermore, there is a strong hybridization of Y d and Sm/Tb/Dy/Yb f states with (Al, Si) p states present between the valence/conduction band regions of both spin types. These states are the major cause for the metallic properties of the materials.

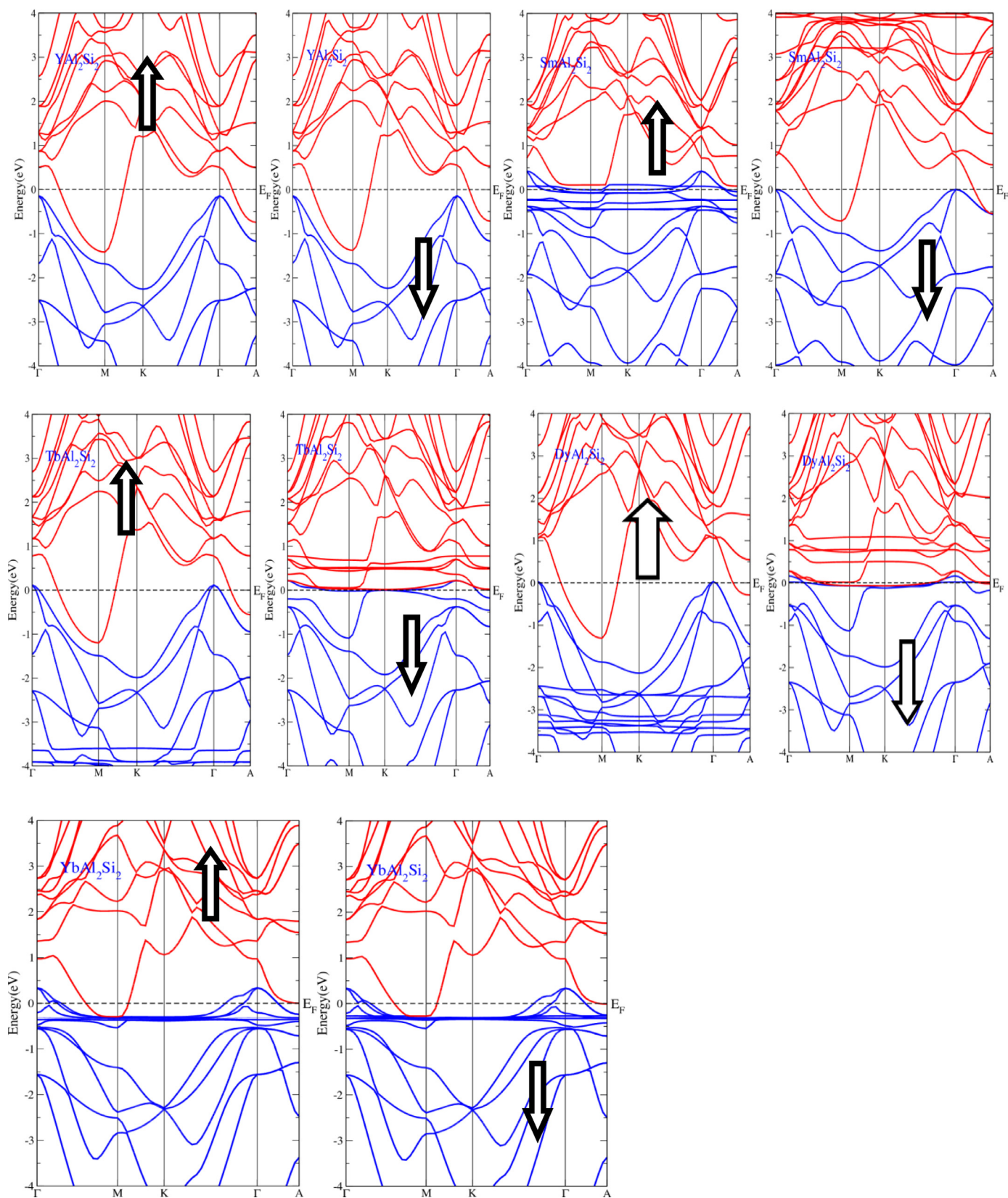


Fig. 2. Band structures of LnAl_2Si_2 ($\text{Ln} = \text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds in Ferromagnetic phase in both spin types.

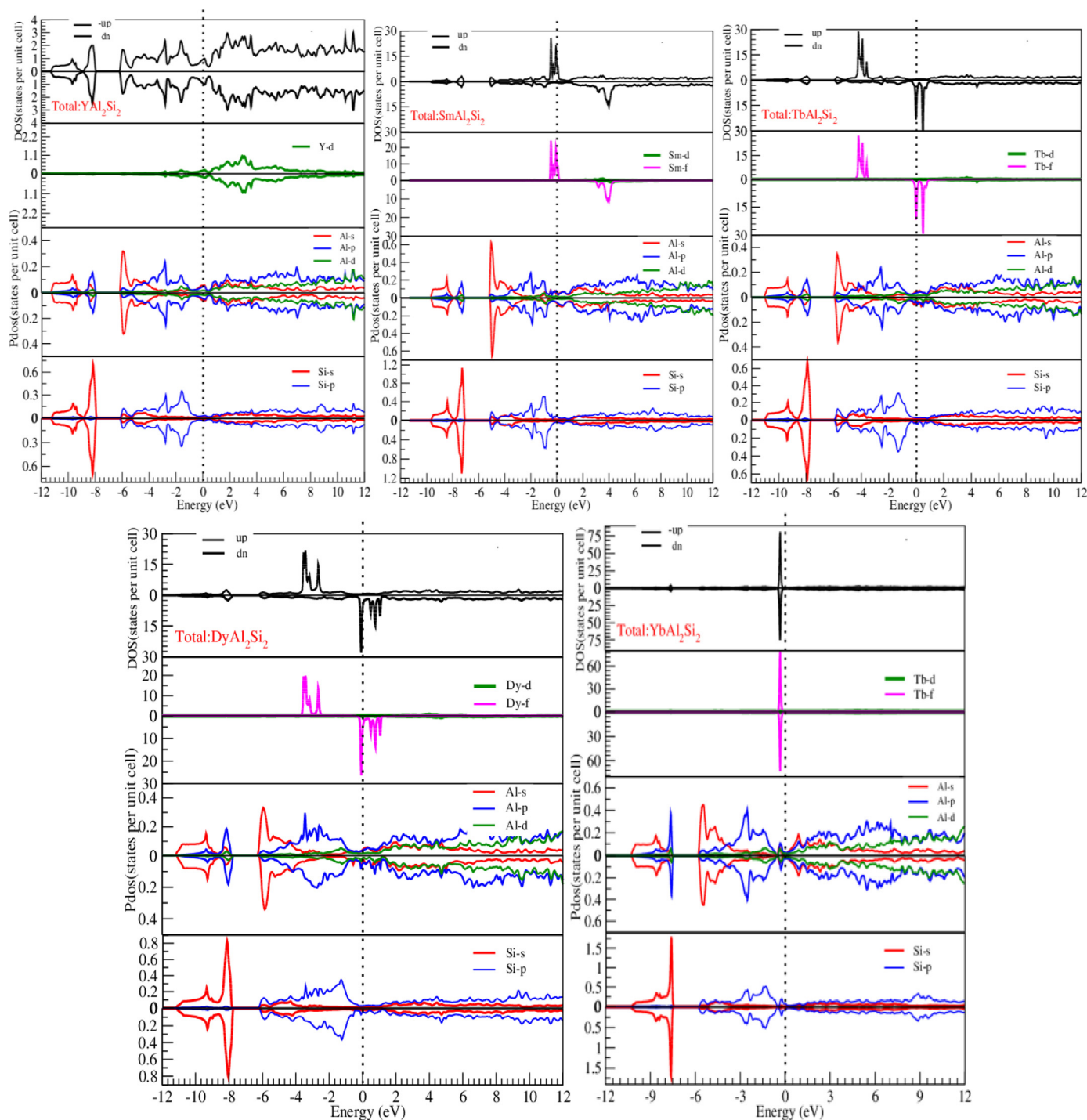


Fig. 3. DOS plots for LnAl_2Si_2 ($\text{Ln} = \text{Y}, \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) compounds in both spin up and down directions.

The major contribution in YAl_2Si_2 compound is due to the lanthanide element Y d state which appears dominantly in the conduction band while minor contribution in valence band region of both spin types and further spread over the entire energy, whereas in the remaining compounds d state disappeared with the appearance of f state clearly seen in ($\text{Ln} = \text{Sm}, \text{Tb}, \text{Dy}, \text{Yb}$) based compounds. Further the Sm/Tb/Dy/Yb f state show peculiar behavior (The noted behavior of these f states $\text{Sm}(4f^6)$ / $\text{Tb}(4f^9)$ / $\text{Dy}(4f^{10})$ / $\text{Yb}(4f^{14})$ for these four compounds are due to the different contributions of f-state electrons) with appearance of state on the Fermi point in up spin and away from the Fermi in the high en-

ergy conduction band region in the down spin channel of SmAl_2Si_2 compound. In addition to this the same sharp f state appears in the up spin away from the Fermi in valence band and remains lie on the Fermi in the down spin state of both TbAl_2Si_2 and DyAl_2Si_2 compounds respectively. Furthermore, follow by the compound YbAl_2Si_2 where a single f state appears at the same lower energy in the valence band region at about -0.7 eV in both spin orientation. Finally, the contribution of Al and Si elements various states are quite similar over the entire energy range in all the investigated compounds with the main dominant contribution of Al/Si-p state with the minor contribution of Al/Si-s and Al-d states

Table 2

Magnetic moments of the interstitial region, individual atoms and total cell for LnAl_2Si_2 ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) compounds using PBE-GGA and GGA+ U methods (in Bohr magnetons μ_B).

Compounds	m^{instr}	$m^{\text{Y/Sm/Tb/Dy/Yb}}$	m^{Al}	m^{Si}	m^{c}
YAl ₂ Si ₂ (PBE-GGA)	0.01717	0.00824	0.00060	-0.00149	0.02362
GGA+ U	0.04523	0.01146	0.00229	-0.00067	0.05992
Exp.	-----	-----	-----	-----	-----
Other calc.					
SmAl ₂ Si ₂ (PBE-GGA)	0.21222	5.70275	-0.00109	-0.01827	5.87625
GGA+ U	0.23883	5.50629	-0.01265	0.01487	5.74956
Exp.	-----	-----	-----	-----	-----
Other calc.					
TbAl ₂ Si ₂ (PBE-GGA)	0.02238	5.71642	-0.00872	-0.00740	5.70654
GGA+ U	0.10761	5.71492	-0.01455	0.01363	5.82069
Exp.	-----	-----	-----	-----	-----
Other calc.					
DyAl ₂ Si ₂ (PBE-GGA)	-0.06055	4.60144	-0.01487	-0.00623	4.49870
GGA+ U	0.04523	0.01146	0.00229	-0.00067	0.05992
Exp.	-----	-----	-----	-----	-----
Other calc.					
YbAl ₂ Si ₂ (PBE-GGA)	-0.00134	0.00956	-0.00747	0.00893	0.01115
GGA+ U	0.02053	-0.22737	-0.00922	0.01017	-0.20493
Exp.	-----	2.57 ^b	-----	-----	-----
Other calc.					

^b Ref:22.

in the valence and conduction bands region of both spin orientations. All the states disappeared in the energy range between -7.5 to -6 eV which is due to the flat band appears in almost all the energy band structure of the compounds as clearly observe in both spin states. Overall, the DOS of reported YAl₂Si₂ compounds shows metallic behavior across the E_f in both spin states.

3.3. Magnetic properties

To get more informative data and comprehensive understanding about the material magnetic properties, we have evaluated the local moments and magnetic interactions in LnAl_2Si_2 ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) compounds through PBE-GGA and GGA + U as noted in Table 2. The non-negative value of the magnetic moment exhibits that the magnetic ground state for LnAl_2Si_2 compounds is ferromagnetic. The calculation through GGA+ U gives higher values for YAl₂Si₂ and SmAl₂Si₂ while smaller for TbAl₂Si₂, DyAl₂Si₂ and YbAl₂Si₂ as compared to other approximation, because it treats localized d/f-shell electrons of Y/(Sm, Tb, Dy, Yb) atoms and slightly increase/decrease its magnetic moment in comparison with PBE-GGA. The total cell magnetic moments are mainly composed of the ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) atoms with small contributions in detail of Al/Si and interstitial site. The Ln atoms have high magnetic moment from other attached atoms in LnAl_2Si_2 compound. As a result of magnetic moment analysis, we have mentioned that the magnetic moment of the lanthanide ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) atoms are higher as compared to Al/Si atoms which is mainly due to the d/f-state of the (Y and Sm, Tb, Dy, Yb) atoms appears dominantly over the entire energy range in both spin types, as reported in the DOS calculations. The fundamental origin of magnetization comes from unoccupied Y- d and (Sm, Tb, Dy, Yb)- f orbital. Moreover, the Y- d and (Sm, Tb, Dy, Yb)- f states are showing the partially filled sub- d/f states. This clearly initiates ferromagnetism in the under reported compounds. On the other side the negative values of magnetic moment define the authentic indication of Al/Si atoms at all sites in the unit cell giving rise to the anti-parallel contribution to the overall ferromagnetic direction due to placement of other constituent's atoms. So the aluminum and silicon site polar-

ized anti-parallel magnetic moment with a negative number and tends to be lower the overall ferromagnetic nature of the materials. In addition to this, the calculated values of the magnetic moment through both approach at interstitial site and total cell for LnAl_2Si_2 compound supports the net magnetic moment, while Al/Si oppose it. From optimization plots in Fig. 1 (a-e) it has cleared that FM is suitable phase for these compounds. Further there is exchange splitting occur in these DOS plots. The Al/Si atoms at all sites oppose because both are aligned anti-parallel to ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) atoms. Furthermore, it will definitely help the magnetic properties if Al/Si atoms aligned parallel to the overall ferromagnetic direction. The opposite sign appears between the magnetic moments of Inst, Ln, Al, Si and total cell exhibits that their valence band electrons interact in anti-ferromagnetic manner. The non-integer values of the magnetic moment confirm that these lanthanide compounds have strong ferromagnetic metallic behavior. The distinctions inside the two noted values are because of the accuracy of GGA+ U over GGA inside the extremely correlated framework shown in Table 2.

4. Conclusions

Detailed Cationic variation for LnAl_2Si_2 ($\text{Ln} = \text{Y, Sm, Tb, Dy, Yb}$) compounds have been discussed under the frame work of density functional theory (DFT). Our reported optimized theoretical lattice constants for the studied material are in good agreement with experimental measurements and we also find that ferromagnetic phase is more stabilize and acceptable in comparison with Nonmagnetic phase. The electronic band structure and density of states (DOS) were investigated for the First time by using a Modified Becke-Johnson exchange potential (mBJ-GGA) scheme. The calculated band structures and density of state (DOS) of understudy compounds show metallic nature due to the overlapping and crossing mechanisms of minima of conduction band (CB) and maxima valance band (VB) across the Fermi level as well as strong hybridization of Y d and Sm/Tb/Dy/Yb f states with (Al, Si) p states in both spin configurations. Lastly, the investigation of magnetic properties defines a strong metallic behavior for all these understudy

ferromagnetic compounds. The fundamental origin of magnetization comes from unoccupied $Y-d$ and $(Sm, Tb, Dy, Yb)-f$ orbital. The non-integer values of the magnetic moment confirm that these lanthanide compounds have strong ferromagnetic metallic behavior. These result shows that the $LnAl_2Si_2$ ($Ln = Y, Sm, Tb, Dy, Yb$) compounds are likely encouraging candidates for advance future magnetic applications especially in the vast area of spintronics.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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